Phase Structure of the Quantum Ising Model in One-Dimensional Space

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Abstract The quantum Ising model is a system of qubits defined on a one-dimensional lattice (a discrete version of one-dimensional space), with an especially simple hamiltonian governing the system's time evolution. It is actually a family of models, parameterized by a real number $\lambda \geq 0$. This family is interesting because it has a nontrivial **phase structure**: the model has a symmetry that is respected by the lowest-energy state when $\lambda < 1$ and that is broken by the lowest-energy state when $\lambda > 1$, a phenomenon called **spontaneous symmetry breaking (SSB)**. These two phases are strictly distinct from each other only when the lattice is infinite. This article defines the model first on a finite lattice and then explores how the strict distinction between the two phases arises when the lattice becomes infinite. The concept of **superselection sectors**, which is important throughout quantum field theory, is one of the keys to understanding how SSB works. The article also explores how this phase structure manages to coexist with another property of the model called **self-duality**, which is a kind of invariance under $\lambda \to 1/\lambda$.

Contents

1 Introduction and context

Many introductions to quantum field theory (QFT) introduce the subject of spontaneous symmetry breaking (SSB) using classical analogies or semiclassical analyses. This article uses the quantum Ising model in one-dimensional space to study SSB without making such compromises. The quantum Ising model is a system of qubits whose behavior is governed by a hamiltonian that depends on a parameter $\lambda \geq 0$, which I'll call the **coupling**. The model can be defined in (the lattice version of) D-dimensional space for any D, but this article focuses on the case $D = 1$, where the calculations are relatively easy to manage.

On an infinite lattice, the model exhibits two distinct phases: a **symmetric** phase when $|\lambda| < 1$, and an **SSB phase** (a phase with spontaneously broken symmetry) when $\lambda > 1$. The case $\lambda = 1$, which sits at the boundary between the symmetric and SSB phases, is called the **critical point**. This article explores the phase structure by first defining the model on a finite lattice and then considering the infinite-lattice limit. Sections 2-4 define two slightly different versions of the model. Sections 5-7 review/introduce some general concepts, and the remaining sections study the models' phase structure.

Much of the literature about the Ising model uses another variant in which both space and time are discretized.[1] The discrete-time variant is often called the two-dimensional Ising model, referring to the number of spacetime dimensions instead of just the number of spatial dimensions.[2] Much of the literature about the Ising model is concerned with its properties at the critical point, where the correlation length diverges and the differences between various discretizations become unimportant.[3] The Ising model has a natural generalization to any number of dimensions, but this article considers only one-dimensional space (2d spacetime), because this is the easiest case with a nontrivial phase structure.

[1] Section IIC in Fradkin and Susskind (1978) and section IV in Kogut (1979) describe the relationship between the discrete- and continuous-time variants. Appendix F in Harlow and Ooguri (2018) reviews a generalization.

[2] After **Wick rotation**, the model can be be reinterpreted as a classical statistical model in 2d space (instead of 2d spacetime). I'm using the name "*quantum* Ising model" to emphasize the conceptual distinction.

[3] This mathematical phenomenon is called **universality**. Article 21916 emphasizes its relevance to QFT.

2 The Hilbert space and qubit operators

The model studied in this article is based on a discretized version of one-dimensional space, which will be called the **lattice**. It will be defined first using a finite number N of points, and then we'll explore what happens when $N \to \infty$.

Choose an integer N. Consider a 2^N-dimensional Hilbert space spanned by vectors $|b\rangle$, one for each N-digit binary number b, with the inner product defined by

$$\langle b|b\rangle = 1 \qquad\qquad \langle b'|b\rangle = 0 \;\text{ if }\; b' \neq b.$$

Any other vector in the Hilbert space is a linear combination of these basis vectors $|b\rangle$ with complex coefficients. For each $n \in \{1, 2, ..., N\}$, define the self-adjoint **Pauli operators** Z_n and X_n by

$$Z_n|b\rangle = \begin{cases} |b\rangle & \text{if the } n\text{th digit is 0} \\ -|b\rangle & \text{if the } n\text{th digit is 1} \end{cases} \qquad\qquad X_n|b\rangle = |b^{(n)}\rangle$$

where $b^{(n)}$ is obtained from b by flipping the nth digit (replacing $0 \leftrightarrow 1$). I'll call them **qubit operators**, because each pair X_n and Z_n defines a **qubit** (article 36176). Using the standard notation

$$[A, B] \equiv AB - BA \qquad\qquad \{A, B\} \equiv AB + BA,$$

these operators satisfy[4]

$$Z_n^2 = 1 \qquad X_n^2 = 1 \qquad \{X_n,\, Z_n\} = 0 \tag{1}$$

$$[X_j,\, X_k] = [X_j,\, Z_k] = [Z_j,\, Z_k] = 0 \qquad \text{whenever } j \neq k.$$

[4]The symbols 1 denotes either the identity operator or the number 1, depending on the context.

3 The hamiltonian

The quantum Ising model on a lattice with N points has several versions, differing from each other in their **boundary conditions** – how the hamiltonian treats the qubits near the endpoints of the lattice. This article will study two different versions.[5] The first one uses the hamiltonian

$$H = -H_X - \lambda H_Z \qquad \text{with} \qquad H_X = \sum_{n=1}^{N} X_n \qquad H_Z = \sum_{n=1}^{N-1} Z_n Z_{n+1}. \tag{2}$$

The second sum can be regarded as a sum over links, where each link is a pair of neighboring sites $(n, n+1)$ in the lattice. I'll call this version the **left-right symmetric** version, because the hamiltonian is symmetric about the center of the lattice (which is a site if N is odd, or the midpoint between two sites if N is even). The second version uses the hamiltonian

$$\hat{H} = -\hat{H}_X - \lambda H_Z \qquad \text{with} \qquad \hat{H}_X = \sum_{n=1}^{N-1} X_n, \tag{3}$$

with H_Z defined as before. This version has a property called **self-duality** even when N is finite (section 21), not just when $N \to \infty$, so I'll call this the **self-dual** version. The two versions differ from each other by a single qubit operator: $H - \hat{H} = X_N$.

Whichever version is used, an eigenstate of the hamiltonian will be called an **energy eigenstate**, and the corresponding eigenvalue will be called the **energy eigenvalue** or just the **energy** (article 22871). The state(s) that have the lowest energy will be called the **ground state(s)**.

[5] This article doesn't consider the version with the **periodic** boundary condition, in which the one-dimensional space wraps back on itself like a circle. That version is attractive because it has translation symmetry even on a finite lattice, but that doesn't necessarily make the model any easier to analyze (footnote 24). Mbeng *et al* (2020) considers periodic and nonperiodic versions of the model.

4 Local observables and the flip-all-bits symmetry

The model associates one qubit with each point in the lattice – with each value of the index $n \in \{1, 2, ..., N\}$. Consecutive index-values represent neighboring points in the lattice, so a string of consecutive index-values represents a region of space. The local observables associated with a given region of space at a given time t are represented by operators in the algebra that is generated by the operators $X_n(t)$ and $Z_n(t)$ for all n in the given region, and the t-dependence is defined by

$$X_n(t) = U^{-1}(t) X_n U(t) \qquad\qquad Z_n(t) = U^{-1}(t) Z_n U(t)$$

with

$$U(t) = \exp(-iHt) \text{ or } \exp(-i\hat{H}t),$$

depending on which version of the model is used.

The model has a symmetry implemented by the unitary operator

$$S \equiv \prod_n X_n, \tag{4}$$

where the product is over all lattice sites. This operator commutes with both versions of the hamiltonian and with each X_n, but it anticommutes with each Z_n. This implies

$$S^{-1} X_n(t) S = X_n(t) \qquad\qquad S^{-1} Z_n(t) S = -Z_n(t), \tag{5}$$

which in turn implies that S implements an **internal symmetry**: it does not mix observables associated with different regions of space at any given time. I'll call it the **flip-all-bits symmetry**, because if $|b\rangle$ is any of the basis states defined in section 2, then $S|b\rangle = |b'\rangle$ where the binary number b' is obtained from b by flipping all of the bits. More generically, this is called a $\mathbb{Z}_2$ symmetry,[6] because the group it generates has only two elements (1 and S, because $S^2 = 1$) and so is isomorphic to the additive group of integers modulo 2.

[6] $\mathbb{Z}$ is standard notation for the additive group of integers, and $\mathbb{Z}_K$ uses addition modulo K.

5 Superselection sectors: the concept

This article is mostly concerned with the limit $N \to \infty$. This section reviews a concept that is central to understanding the model's interpretation in that limit.

Any time the state ends up in the form $|\psi\rangle = \sum_n |\psi_n\rangle$ where the terms $|\psi_n\rangle$ cannot be mixed with each other by any of the operators representing future observables that could feasibly be measured, we might as well replace the original superposition $|\psi\rangle$ with one of those distinguished terms $|\psi_n\rangle$, because we can only experience one of them.[7] This is the criterion we use, either explicitly or implicitly, to recognize the occurrence of a *measurement* in quantum theory (article 03431). If the distinguished terms $|\psi_n\rangle$ are eigenstates of an observable with distinct eigenvalues, then we say that the observable has been measured, and the state-replacement rule tells us to project the original state onto one of those eigenstates. The criterion doesn't tell us *which* one, nor does it tell us exactly when the projection should be applied, but the criterion works well enough in practice: it is as predictive as it needs to be, for everything that real experiments have actually been able to do.

The same criterion plays an important role in understanding SSB, illustrated here by the quantum Ising model in the limit $N \to \infty$. In that limit, the Hilbert space defined in section 2 is much too big: it encompasses many different **superselection sectors**, subspaces that cannot be mixed with each other by any local[8] observables – observables associated with bounded regions of space at a given time. In this case, the criterion reviewed in the previous paragraph is unambiguous: any state of the form $|\psi\rangle = \sum_n |\psi_n\rangle$, where the terms $|\psi_n\rangle$ belong to different superselection sectors, might as well be replaced by one of those terms $|\psi_n\rangle$.

[7] The statement about *experience* applies to models that are meant to be good representations of real systems. This article is using the Ising model only as a **toy model**: it's not intended to have practical applications to any real system, but we still hold it to at least some of the same principles, because the purpose of studying the toy model is to develop intuition about the consequences of those principles.

[8] I'm specifying *local* observables here because other observables are defined in terms of these as part of the definition of the limit $N \to \infty$, using an approach like Witten (2021) describes in section 2.2.

6 Choosing a superselection sector

When applying the state-replacement rule in the wake of a measurement, quantum theory doesn't tell us which of the possible outcomes should be selected. It only assigns probabilities to them. We can't be sure which one we should chose until the measurement occurs in the real world and we experience one of the outcomes. We can only do this *after* the measurement occurs. In contrast, when we choose a superselection sector, we are choosing the set of allowed *initial* states.

When $N \to \infty$, the Hilbert space defined in section 2 encompasses many different superselection sectors.[9] Which one should we choose? We can think of this as part of deciding which *model* we should choose, and the answer is the same: we should choose whichever one agrees with the results of real experiments. That might be too much to expect when studying a *toy model* like the one we're studying in this article, but we can still apply some general guidelines based on experience with more realistic models.

One guideline is the **spectrum condition**, which says that the spectrum of the hamiltonian should have a finite lower bound (article 22871). In the quantum Ising model, the spectrum condition is automatic when N is finite. To enforce it when $N \to \infty$, we can substract the N-dependent lowest energy from the hamiltonian before taking the limit.[10] We can choose one of the states that asymptotically approaches the lowest possible energy (which is now zero), retaining all states that can be obtained from that one by applying finite[11] numbers of qubit operators (section 2), but discarding states that are orthogonal to all of those. The resulting Hilbert space might still encompass more than one superselection sector, but at least they all satisfy the spectrum condition.

[9] Even if we didn't know this, we would still know that the Hilbert space is too big, because the Hilbert space used to represent observables in quantum theory is normally supposed to be **separable**: every orthonormal basis should be countable (article 90771). The Hilbert space defined in section 2 is not separable when $N = \infty$.

[10] This is illustrated in last picture in section 13.

[11] Sections 2.2 and 3.3 in Witten (2021) explain how choosing a separable subspace relates to choosing a topology in which to complete the algebra of observables.

7 Spontaneous symmetry breaking: definition

In some cases, restricting the model to a single superselection sector that satisfies the spectrum condition breaks what would have otherwise been a symmetry of the model. This is called **spontaneous symmetry breaking (SSB)**.[12] The quantum Ising model in one-dimensional space exhibits this phenomenon with respect to the flip-all-bits symmetry that was defined in section 4.

In the Ising model, *perfect* SSB – with perfect superselection sectors – requires $N \to \infty$. That's the subject of the remaining sections in this article, but the related concept of *effective* SSB is more relevant for real-world systems. As emphasized in section 5, any time a system ends up in a state of the form $|\psi\rangle = \sum_n |\psi_n\rangle$ where the terms $|\psi_n\rangle$ cannot be mixed with each other by any of the operators representing future observables that could *feasibly* be measured, we might as well replace the original superposition $|\psi\rangle$ with one of those distinguished terms $|\psi_n\rangle$. If the model has a symmetry that mixes these distinguished terms $|\psi_n\rangle$ with each other, then applying the state-replacement rule breaks that symmetry. Because of the qualifier *feasibly*, this can occur even if the size of the system (analogous to the value of N) is finite.[13]

This article uses the quantum Ising model as a toy model, not intended to be a good representation of any real system. In a toy model, the condition "could feasibly be measured" does not have any clear meaning. That's why this article focuses on *perfect* SSB. Keep in mind, though, that in more realistic models, *perfect* SSB is interesting mainly because it ensures that *effective* SSB will occur when the system is cool enough.

[12] SSB is often regarded as a consequence of requiring the ground state $\rho(\cdots) \equiv \langle g|\cdots|g\rangle/\langle g|g\rangle$ to satisfy the **cluster property**, which roughly says that $\rho\big(Q(x)Q'(y)\big) \to \rho\big(Q(x)\big)\rho\big(Q'(y)\big)$ as $|x-y| \to \infty$. In words: it says that ground-state correlations between observables that are far away from each other become negligible as the distance between them goes to infinity. The relationship between the cluster property and the superselection-sectors criterion is not addressed in this article. (This article doesn't consider correlation functions.)

[13] Sections 1.6-1.7 in Landsman (2013) present a related-but-different perspective.

8 Outline of the remaining sections

Sections 3 defined two slightly different hamiltonians, which give two slightly different versions of the quantum Ising model when N is finite. The difference between them doesn't really matter in the limit $N \to \infty$, but it does matter when N is finite. Understanding how the SSB phase emerges in the limit $N \to \infty$ in both versions can be enlightening, so this article analyzes both of them. Here's an outline:

- Sections 12-20 analyze the left-right symmetric version of the model, with hamiltonian (2). The analysis of this model will confirm what section 1 said about the phase structure: in the limit $N \to \infty$, the flip-all-bits symmetry (5) is spontaneously broken if and only if $\lambda > 1$.

- Sections 21-24 analyze the other version of the model, the one that uses the hamiltonian (3). For arbitrary N, this version of the model is **self-dual**, which is a kind of invariance under $\lambda \to 1/\lambda$.

Both versions of the model should make the same predictions when $N \to \infty$, but the self-duality of the second version might seem incompatible with the phase structure of the first version, where the cases $\lambda < 1$ and $\lambda > 1$ are distinguished from each other by qualitatively different properties. Section 22 decomposes this paradox into three pieces, and sections 22-24 explain how each piece is resolved.

9 The zero-coupling case

Start with the left-right symmetric hamiltonian (2), which will occupy our attention from now through section 20.

When N is large, constructing the ground state(s) explicitly is typically difficult, but it becomes easy in two limiting cases: $\lambda = 0$, and $\lambda \to \infty$. This section considers the $\lambda = 0$ case, and the next section considers $\lambda \to \infty$.

When $\lambda = 0$, the left-right symmetric hamiltonian (2) reduces to H_X. The operator H_X is a sum of single-qubit operators, so the qubits don't interact with each other in this case. The ground state is

$$|g\rangle \equiv \sum_b |b\rangle, \tag{6}$$

where the sum is over all N-digit binary numbers b, because this is an eigenstate of every X_n with eigenvalue 1.[14] The state (6) is an eigenstate of each X_n with eigenvalue 1, so this state has energy $-N$, which is the lowest possible for the hamiltonian H_X.

Other energy eigenstates can be constructed by multiplying $|g\rangle$ by a product of one or more Zs. The result is again an eigenstate of each X_n, now with eigenvalues ± 1 depending on whether a factor of Z_n was included in the product. Altogether, this gives a set of 2^N energy eigenstates, because each of the N operators Z_n may be either included in the product or not. This is enough states to span the Hilbert space, so all other energy eigenstates must be superpositions of these.[15] The energy eigenvalues are all integers, either all even integers or all odd integers, depending on whether N is even or odd. This is a prominent feature of the $\lambda = 0$ side of the pictures shown in section 13.

[14] Recall that X_n flips the nth bit, so X_n merely permutes the summands $|b\rangle$ with each other without changing their coefficients.

[15] A superposition of two energy eigenstates with equal energies is another energy eigenstates with that same energy.

10 The infinite-coupling limit

To define the limit $\lambda \to \infty$, we can use the rescaled[16] hamiltonian $\lambda^{-1}H$. In the limit $\lambda \to \infty$, the rescaled hamiltonian reduces to H_Z. The all-0s and all-1s states

$$|000\cdots000\rangle \qquad\qquad |111\cdots111\rangle$$

are *both* ground states.[17] They both have the same energy, namely $-(N-1)$, which is the negative of the number of links. This is the lowest eigenvalue of H_Z.

Other energy eigenstates can be constructed by multiplying either of these two ground states by a product of one or more Xs. The result is again an eigenstate of each term in H_Z, now with eigenvalues ±1 depending on which factors of X_n were included in the product. Multiplying by *all* of the X_ns exchanges the two ground states with each other.

Altogether, this gives a set of 2^N energy eigenstates, which is enough to span the Hilbert space, so all other energy eigenstates must be superpositions of these. The energy eigenvalues are all integers, either all even integers or all odd integers, depending on whether N is even or odd. For the original hamiltonians H and $\hat{H}$, without the overall rescaling factor λ^{-1}, these integers describe the asymptotic *slopes* of the energy-versus-λ graphs for large λ. These slopes are a prominent feature of the pictures shown in section 13.

[16]This rescaling is perfectly legal. The overall proportionality factor is not important, because changing it is the same as changing the unit of energy or the unit of time. We could have defined the hamiltonian more generally as $H \propto -\cos(\phi)H_X - \sin(\phi)H_Z$, and then the special cases $\phi = 0$ and $\phi = \pi/2$ correspond to $\lambda = 0$ and $\lambda \to \infty$, respectively, aside from the choice of units.

[17]The all-0s state is an eigenstate of every Z_n with eigenvalue 1, and the all-1s state is an eigenstate of every Z_n with eigenvalue -1, so both states are eigenstates of every Z_nZ_{n+1} with eigenvalue 1.

11 Spontaneous symmetry breaking: preview

The previous section showed that in the limit $\lambda \to \infty$, the model has two ground states – the all-0s state and the all-1s state – that are exchanged with each other by the flip-all-bits symmetry. This is true for arbitrary N.

In the limit $N \to \infty$, local observables cannot mix the all-0s and all-1s states with each other: no matter how we change the states inside a finite region of space (finite number of lattice sites), they will still be orthogonal to each other because of their opposite bit-values arbitrarily far away. This illustrates SSB.

This illustration is almost too simple, though, because these two states are both eigenstates of all of the single-qubit operators Z_n. When λ is finite, none of the ground state(s) are eigenstates of *any* single-qubit operators (except trivial operators that are proportional to the identity operator). Instead, the qubits are all entangled with each other, to a degree that increases as λ decreases toward the critical value $\lambda = 1$. Even if we had an explicit expression of the form $\sum_b c_b|b\rangle$ for each ground state, with known coefficients c_b, diagnosing SSB directly from those expressions would be difficult.

Section 18 uses a less direct but easier approach. The result is that when $N \to \infty$, the flip-all-bits symmetry is spontaneously broken for all $\lambda > 1$. It remains unbroken for $\lambda < 1$.

12 Energy eigenstates on a two-site lattice

When $N = 2$, the sums in the hamiltonian (2) reduce to

$$H_X = X_1 + X_2 \qquad\qquad H_Z = Z_1 Z_2,$$

so the hamiltonian reduces to

$$H = -(X_1 + X_2) - \lambda Z_1 Z_2.$$

The Hilbert space is only 4-dimensional (only two qubits), so the complete set of energy eigenstates is easy to determine analytically. Here are the results:

Eigenvalue	Eigenstate
$\sqrt{\lambda^2+4}$	$\|00\rangle + \|11\rangle + \frac{1}{2}\left(-\lambda - \sqrt{\lambda^2+4}\right)\left(\|01\rangle + \|10\rangle\right)$
λ	$\|01\rangle - \|10\rangle$
$-\lambda$	$\|00\rangle - \|11\rangle$
$-\sqrt{\lambda^2+4}$	$\|00\rangle + \|11\rangle + \frac{1}{2}\left(-\lambda + \sqrt{\lambda^2+4}\right)\left(\|01\rangle + \|10\rangle\right)$

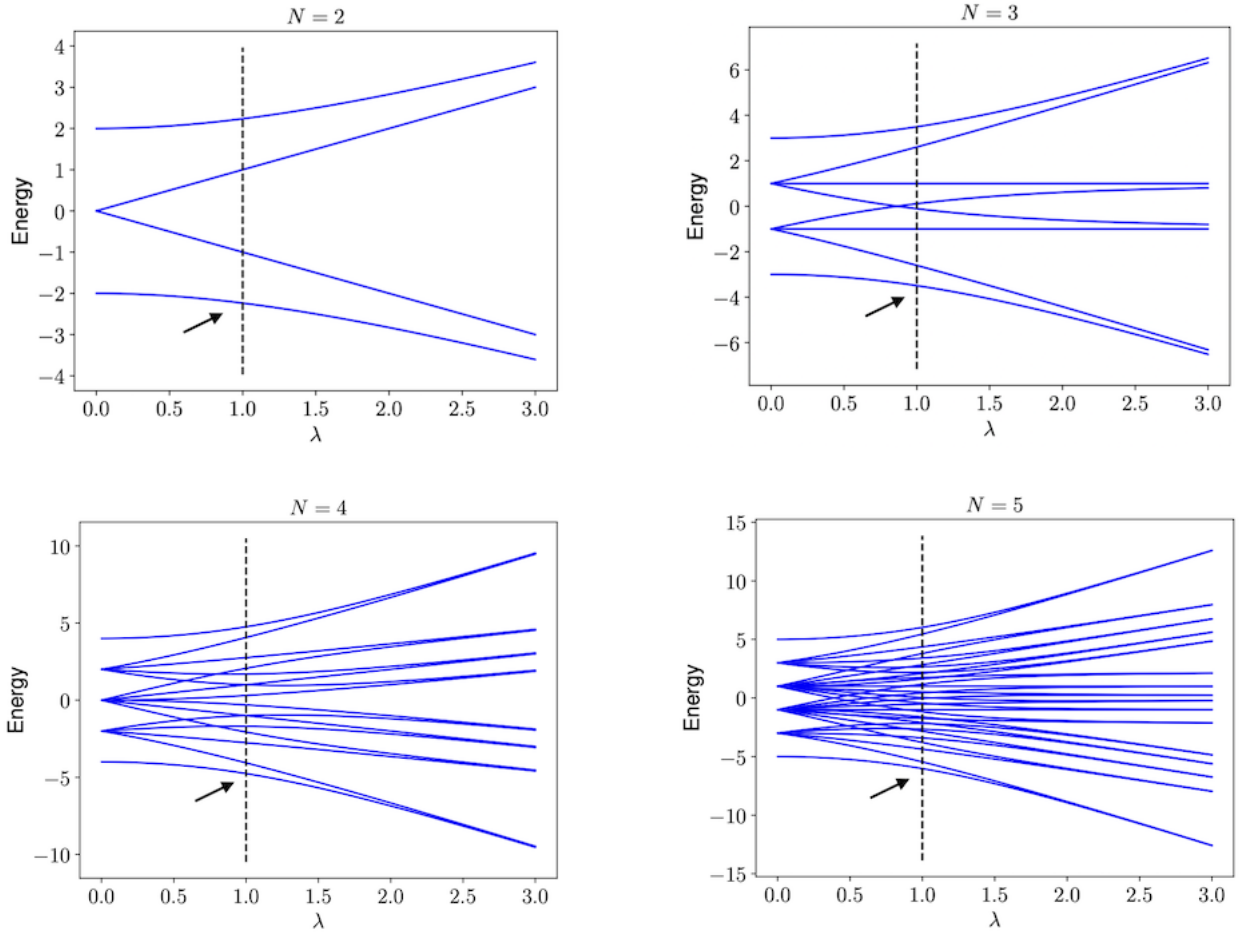
in order from highest to lowest energy. The ground state is the last entry in this list. The results tabulated above are consistent with the observations in sections 9 and 10. When $\lambda = 0$, only one state has the lowest energy, namely $|00\rangle+|11\rangle+|01\rangle+|10\rangle$, and this state is invariant under the flip-all-bits symmetry. When $\lambda \to \infty$, the two lowest energies of the rescaled hamiltonian $\lambda^{-1}H$ both become equal to -1. Use

$$\lim_{\lambda\to\infty} \frac{-\lambda + \sqrt{\lambda^2+4}}{\lambda} = 0$$

to see that the corresponding energy eigenstates become $|00\rangle \pm |11\rangle$, and since their energies are equal, the set of lowest-energy states includes $|00\rangle$ and $|11\rangle$, as observed in section 10.

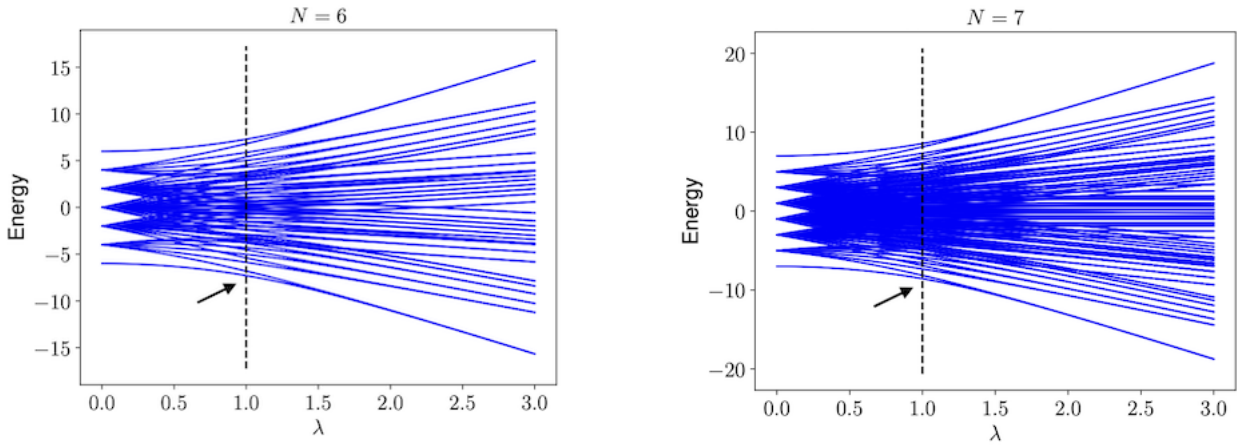
13 Energy spectrum on small lattices

Sections 15-(20) will show how to calculate the spectrum of energies exactly, on a lattice with an arbitrary number N of sites. For small N, the energy spectrum may also be determined numerically. Here are a few examples:[18,19]

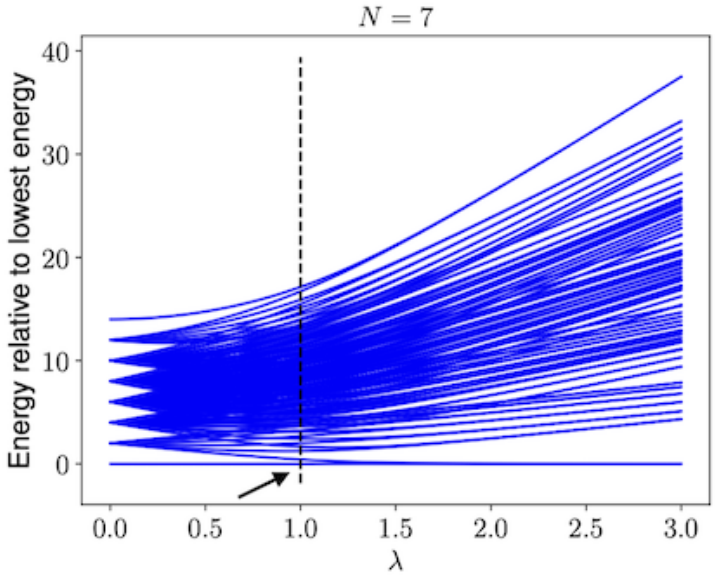


[18] These results were generated using Python. The pictures are slightly blurry because I reduced the resolution to keep the file size under control. The Python script is posted here: https://cphysics.org/extras/81040a.html

[19] These spectra are evidently invariant under a sign-change of the energy. To explain this, let π_Z be the product of all of the Z_ns, and let π_X be the product of all of the X_ns with n even. Then $\pi_X\pi_Z$ anticommutes with every term in the hamiltonian, so if $|\psi\rangle$ is an energy eigenstate, then so is $\pi_X\pi_Z|\psi\rangle$, with the opposite sign for the energy.



Here's the $N = 7$ case again, this time showing the energies relative to the lowest energy:



The arrow calls attention to where the lowest and second-lowest energies cross $\lambda = 1$. Section 18 will show that this is the threshold between the symmetric and SSB phases when $N \to \infty$.

14 More notation

To streamline the analysis in the following sections, let I denote the $N \times N$ identity matrix, which has components

$$I_{jk} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{otherwise,} \end{cases}$$

and let T denote the **translation** matrix with components

$$T_{jk} = \begin{cases} 1 & \text{if } j + 1 = k, \\ 0 & \text{otherwise.} \end{cases}$$

For $N = 5$, the matrices I and T are

$$I = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

In this article, if A is an operator on the Hilbert space, then its adjoint will be denoted A^*, as in article 74088. Given a matrix M whose individual components M_{jk} are either complex numbers or operators on the Hilbert space, the notation $M^\dagger$ will be used for the matrix with components

$$(M^\dagger)_{jk} = (M_{kj})^*$$

(notice the transpose), where the right-hand side is the complex conjugate of M_{kj} if it's a complex number, or the adjoint of M_{kj} if it's an operator.

15 How to diagonalize the hamiltonian, part 1

The next goal is to diagonalize[20] the left-right symmetric version of the hamiltonian, equation (2), repeated here for convenience:

$$H = -\sum_{n=1}^{N} X_n - \lambda \sum_{n=1}^{N-1} Z_n Z_{n+1}. \tag{7}$$

Define

$$A_n \equiv Z_n S_{n+1} \qquad\qquad B_n \equiv -iZ_n S_n \tag{8}$$

with[21]

$$S_n \equiv \prod_{k \geq n} X_k \qquad\qquad S_{N+1} \equiv 1. \tag{9}$$

The operators (8) are self-adjoint.[22] Use equations (1) to get

$$\{A_j, A_k\} = 2\delta_{jk} \qquad\qquad \{A_j, B_k\} = 0 \qquad\qquad \{B_j, B_k\} = 2\delta_{jk}. \tag{10}$$

This is a **Clifford algebra**, so A_n and B_n will be called **Clifford operators**. Each of these Clifford operators is a nonlocal[23] combination of the original qubit operators X, Z. The nonlocality is evident in equation (9). Use[24]

$$X_n = iA_n B_n \qquad\qquad Z_n Z_{n+1} = -iA_n B_{n+1} \tag{11}$$

and use the fact that the As and Bs anticommute with each other to write (7) as

$$H = -i \sum_{n=1}^{N} A_n B_n + i\lambda \sum_{n=1}^{N-1} A_n B_{n+1},$$

[20] I'm using the word *diagonalize* as an abbreviation for finding all of the eigenvectors and eigenvalues.

[21] Mnemonic: S stands for a *string* of Xs, like in (4).

[22] This is why the factor of i is included in B_n.

[23] Here, *nonlocal* means not contained within any small neighborhood.

[24] This works well because the lattice has an endpoint that provides a natural point at which the string of factors of X in the definitions (8) can begin, in contrast to the periodic version that was mentioned in footnote 5.

which may also be written

$$H = \frac{i}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} (B_j M_{jk}^{\dagger} A_k - A_j M_{jk} B_k) \tag{12}$$

where M_{jk} are the components of the $N \times N$ matrix

$$M = I - \lambda T, \tag{13}$$

with I and T defined as in section 14. For $N = 5$, the matrix (13) is

$$M = \begin{bmatrix} 1 & -\lambda & 0 & 0 & 0 \\ 0 & 1 & -\lambda & 0 & 0 \\ 0 & 0 & 1 & -\lambda & 0 \\ 0 & 0 & 0 & 1 & -\lambda \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

We can write H even more concisely as

$$H = \frac{i}{2} (B^{\dagger} M^{\dagger} A - A^{\dagger} M B) \tag{14}$$

with

$$A \equiv \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{bmatrix} \qquad\qquad B \equiv \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_N \end{bmatrix}.$$

The matrices A and B both have size $N \times 1$, and each of their components is an operator on the Hilbert space. If the two matrices A and B are concatenated into a single matrix of size $2N$, then equation (14) can also be written like this:

$$H = \frac{i}{2} \begin{bmatrix} A \\ B \end{bmatrix}^{\dagger} \begin{bmatrix} 0 & -M \\ M^{\dagger} & 0 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{15}$$

In the middle matrix, each "0" represents an all-zeros matrix of size $N \times N$.

16 Interlude: some matrix math

Thanks to equation (15), the task of diagonalizing the hamiltonian has essentially been reduced to the task of diagonalizing the self-adjoint matrix

$$i\begin{bmatrix} 0 & -M \\ M^\dagger & 0 \end{bmatrix}, \tag{16}$$

with M given by equation (13). That's progress, because the structure of this matrix is simpler than the structure of the hamiltonian, when the hamiltonian is viewed as a matrix acting on the 2^N-dimensional Hilbert space. This section explains how to relate the eigenvectors[25] and eigenvalues of any matrix of the form (16) to the eigenvectors and eigenvalues of the positive-definite matrices $M^\dagger M$ and $MM^\dagger$. This section does not use equation (13).

Here's some useful notation: for any nonzero N-component vector u, define

$$m(u) \equiv \sqrt{\frac{(Mu)^\dagger Mu}{u^\dagger u}} = \sqrt{\frac{u^\dagger M^\dagger Mu}{u^\dagger u}}.$$

If u is an eigenvector of $M^\dagger M$, then $m^2(u)$ is the corresponding eigenvalue. We will see that the eigenvalues of (16) are $\pm m(u)$.

The matrices $M^\dagger M$ and $MM^\dagger$ don't necessarily have the same eigenvectors, but they do have the same eigenvalues, and they have the same *numbers* of linearly independent eigenvectors corresponding to each of those eigenvalues. This will be proved first for the nonzero eigenvalues, and then for the zero eigenvalues.

To prove that $M^\dagger M$ and $MM^\dagger$ have the same number of linearly independent eigenvectors for each nonzero eigenvalue, suppose that u is an eigenvector of $M^\dagger M$ with eigenvalue $m^2(u)$. Then Mu is clearly an eigenvector of $MM^\dagger$ with the same eigenvalue $m^2(u)$. If u and u' are two linearly independent eigenvectors of $M^\dagger M$ with the same *nonzero* eigenvalue $m^2(u) \neq 0$, then Mu and Mu' are linearly independent, because $M^\dagger Mu \propto u$ and $M^\dagger Mu' \propto u'$ are. Similarly, if $\tilde{u}$ is an eigenvector

[25] The word **vector** will be used here for any single-column matrix whose components are ordinary complex numbers (not operators).

of $MM^\dagger$, then $M^\dagger\tilde{u}$ is an eigenvector of $M^\dagger M$ with the same eigenvalue, and this construction again preserves linear independence if the eigenvalue is nonzero. Altogether, this shows that $M^\dagger M$ and $MM^\dagger$ have the same nonzero eigenvalues, and they have the same numbers of linearly independent eigenvectors corresponding to each nonzero eigenvalue.

The matrices $M^\dagger M$ and $MM^\dagger$ are both self-adjoint, so they must each have exactly N linearly independent eigenvectors. The previous paragraph already showed that they have the same numbers of eigenvectors with nonzero eigenvalues, so they must also have the same number of eigenvectors with eigenvalue zero.[26] Altogether, since $M^\dagger M$ and $MM^\dagger$ have the same number of linearly independent eigenvectors with each eigenvalue, including zero.

Let U denote a set of N mutually orthogonal eigenvectors of $M^\dagger M$. The preceding results imply that we can choose a corresponding set $\tilde{U}$ of N mutually orthogonal unit eigenvectors of $MM^\dagger$ and a one-to-one correspondence between U and $\tilde{U}$ with these properties:[27]

- If $u \in U$ and $m(u) \neq 0$, then the corresponding $\tilde{u} \in \tilde{U}$ is $\tilde{u} = Mu/m(u)$.
- If $u \in U$ and $m(u) = 0$, then the corresponding $\tilde{u} \in \tilde{U}$ satisfies $MM^\dagger\tilde{u} = 0$.

Given such sets U and $\tilde{U}$ with this correspondence between them, every $2N$-component vector of the form

$$\begin{bmatrix} \pm\tilde{u} \\ iu \end{bmatrix}$$

is an eigenvector of the matrix (16) with corresponding eigenvalue $\pm m(u)$:

$$i\begin{bmatrix} 0 & -M \\ M^\dagger & 0 \end{bmatrix}\begin{bmatrix} \tilde{u} \\ iu \end{bmatrix} = m(u)\begin{bmatrix} \tilde{u} \\ iu \end{bmatrix} \qquad i\begin{bmatrix} 0 & -M \\ M^\dagger & 0 \end{bmatrix}\begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix} = -m(u)\begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix}. \quad (17)$$

[26] This inference assumes that N is finite. If $N = \infty$, then $M^\dagger M$ and $MM^\dagger$ can have different numbers of linearly independent eigenvectors with eigenvalue zero. Example: if T is defined as in section 14, then $T^\dagger T$ has one zero eigenvalue when $N = \infty$, but $TT^\dagger$ doesn't have any.

[27] If more than one $u \in U$ has eigenvalue zero, then we must make arbitrary choices to establish a one-to-one correspondence with $\tilde{U}$.

To check this when $m(u) = 0$, us the fact that the conditions $M^\dagger M u = 0$ and $M M^\dagger \tilde{u} = 0$ imply $(Mu)^\dagger M u = 0$ and $(M^\dagger \tilde{u})^\dagger M^\dagger \tilde{u} = 0$, respectively, which then imply $Mu = 0$ and $M^\dagger \tilde{u} = 0$.

Altogether, the construction described above gives one pair of eigenvectors of (16) for each $u \in U$, and all of these eigenvectors of (16) are orthogonal to each other. The set U has N elements, so this gives a complete set of $2N$ mutually orthogonal eigenvectors of (16). One important consequence of this is that the matrix (16) may be written

$$i \begin{bmatrix} 0 & -M \\ M^\dagger & 0 \end{bmatrix} = \sum_{u \in U} m(u) \left(\begin{bmatrix} \tilde{u} \\ iu \end{bmatrix} \begin{bmatrix} \tilde{u} \\ iu \end{bmatrix}^\dagger - \begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix} \begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix}^\dagger \right) \tag{18}$$

if the us and $\tilde{u}$s are normalized so that

$$\begin{bmatrix} \tilde{u} \\ iu \end{bmatrix}^\dagger \begin{bmatrix} \tilde{u} \\ iu \end{bmatrix} = \begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix}^\dagger \begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix} = 1, \tag{19}$$

which will be assumed from now on. The next section uses the identity (18) as a step toward diagonalizing the hamiltonian.

17 How to diagonalize the hamiltonian, part 2

When M is given by (13), the matrix $M^\dagger M$ has only real-valued components. The eigenvalues of $M^\dagger M$ are real-valued, too, so we can choose the eigenvectors in the set U (defined in section 16) to have only real-valued components, and similarly for the set $\tilde{U}$. If these vectors are also normalized as in (19), then equations (10) imply that the operators[28]

$$c(u) \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} A \\ B \end{bmatrix}^\dagger \begin{bmatrix} -\tilde{u} \\ iu \end{bmatrix} \qquad \text{with } u \in U \tag{20}$$

satisfy

$$\{c(u), c(u')\} = 0 \qquad \{c(u), c^*(u')\} = \delta(u, u') \tag{21}$$

with

$$\delta(u, u') \equiv \begin{cases} 1 & \text{if } u = u' \\ 0 & \text{otherwise.} \end{cases}$$

These are the canonical anticommutation relations for a set of fermion modes, one for each $u \in U$, so the operators $c(u)$ will be called **fermion operators**.[29] Substitute (18) into (15) and use (21) to get this expression for the hamiltonian:

$$\begin{aligned} H &= \frac{1}{2} \sum_{u \in U} m(u) \big(c^*(u) c(u) - c(u) c^*(u) \big) \\ &= \frac{1}{2} \sum_{u \in U} m(u) \big(2 c^*(u) c(u) - 1 \big). \end{aligned}$$

To see why this is useful, define $|g\rangle$ to be the state satisfying

$$c(u)|g\rangle = 0 \qquad \text{for all } u \in U. \tag{22}$$

[28] The factor $1/\sqrt{2}$ here compensates for the factor of 2 in equations (10).

[29] Molignini (2013) gives a pedagogical review of the Majorana-fermion representation of the Ising model.

Then $|g\rangle$ has the lowest possible energy, and all other energy eigenstates can be written

$$\prod_{u\in V} c^*(u)|g\rangle$$

with corresponding eigenvalue

$$E(V) \equiv \sum_{u\in V} m(u) - \frac{1}{2}\sum_{u\in U} m(u). \tag{23}$$

Each subset $V \subset U$ gives a different eigenstate. The set U has N elements, so the number of distinct subsets $V \subset U$ is 2^N. This matches the number of dimensions of the Hilbert space, as it should, because when the Hilbert space is finite-dimensional, it should have a basis consisting of eigenstates of the hamiltonian.[30]

Equation (23) gives the complete set of energy eigenvalues of the hamiltonian (2), one for each subset $V \subset U$. The numbers $m(u)$ are the positive square roots of $m^2(u)$, and the numbers $m^2(u)$ are the eigenvalues of the matrix

$$M^\dagger M = I - \lambda(T^\dagger + T) + \lambda^2 T^\dagger T, \tag{24}$$

or of the matrix

$$MM^\dagger = I - \lambda(T^\dagger + T) + \lambda^2 TT^\dagger, \tag{25}$$

with M defined by (13). The problem of determining the complete energy spectrum has been reduced to determining the eigenvalues of the matrix (24) (or (25)), which has a relatively simple structure. This will be done in sections 19-(20).

[30]This is not necessarily true when the Hilbert space is infinite-dimensional.

18 Spontaneous symmetry breaking: derivation

This section shows that in the limit $N \to \infty$, the model with $\lambda > 1$ has two superselection sectors that both satisfy the spectrum condition and that are exchanged with each other by the flip-all-bits symmetry defined in section 4. This is spontaneous symmetry breaking. The analysis will be done in three steps:

1. Show that the model has two linearly independent ground states.
2. Show that this 2d space of ground states includes two states, say $|g_+\rangle$ and $|g_-\rangle$, that are exchanged with each other by the flip-all-bits symmetry.
3. Show that the ground states $|g_\pm\rangle$ cannot be mixed with each other by any local observables.

If these conditions are satisfied, then we can generate the required pair of superselection sectors by acting on $|g_+\rangle$ or $|g_-\rangle$, respectively, with the algebra of local observables.[31]

The first step is to show that the model has two linearly independent ground states. According to (23), the difference between the two lowest eigenvalues of H is zero if and only if one of the quantities $m(u)$ is zero. To see when this happens, consider the case $N = 5$, from which the pattern for arbitrary N should be clear. When $N = 5$, the matrix (24) is

$$M^\dagger M = \begin{bmatrix} 1 & -\lambda & 0 & 0 & 0 \\ -\lambda & 1+\lambda^2 & -\lambda & 0 & 0 \\ 0 & -\lambda & 1+\lambda^2 & -\lambda & 0 \\ 0 & 0 & -\lambda & 1+\lambda^2 & -\lambda \\ 0 & 0 & 0 & -\lambda & 1+\lambda^2 \end{bmatrix}. \tag{26}$$

[31] Section 2.2 in Witten (2021) explains how the algebra may be completed to include other observables (not just the local ones) after one of the ground states is selected.

The vector

$$w = \begin{bmatrix} 1 \\ 1/\lambda \\ 1/\lambda^2 \\ 1/\lambda^3 \\ 1/\lambda^4 \end{bmatrix} \tag{27}$$

satisfies

$$M^\dagger M w = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1/\lambda^4 \end{bmatrix},$$

so the vector w is not quite an eigenvector, but for any $\lambda > 1$, it approaches an eigenvector with eigenvalue zero as $N \to \infty$.[32,33] For any finite N, the ground state $|g\rangle$ is unique. We just learned that if $\lambda > 1$, then $M^\dagger M$ has an eigenvector $u_0 \in U$ for which $m(u_0) \to 0$ as $N \to \infty$, so the state $c^*(u_0)|g\rangle$ becomes another ground state in that limit. The ground states $|g\rangle$ and $c^*(u_0)|g\rangle$ are linearly independent, so this completes step 1.

For reference in step 3, below, the $N = 5$ version of the matrix (25) is

$$MM^\dagger = \begin{bmatrix} 1+\lambda^2 & -\lambda & 0 & 0 & 0 \\ -\lambda & 1+\lambda^2 & -\lambda & 0 & 0 \\ 0 & -\lambda & 1+\lambda^2 & -\lambda & 0 \\ 0 & 0 & -\lambda & 1+\lambda^2 & -\lambda \\ 0 & 0 & 0 & -\lambda & 1 \end{bmatrix}. \tag{28}$$

The matrix (28) is like (26) but with the index order reversed, so we can apply the

[32] It also approaches an eigenvector with eigenvalue zero in the limit $\lambda \to \infty$, even if N is finite, as anticipated in section 10.

[33] This doesn't work when $|\lambda| < 1$, because in that case the $N \to \infty$ version of the vector w is not normalizable, so it we can't rescale it to give a unit eigenvector of $M^\dagger M$. This is one indication that $\lambda = 1$ is a threshold between two qualitatively different phases.

same kind of reasoning as before: if $\lambda > 1$, then the vector

$$\tilde{w} = \begin{bmatrix} \vdots \\ 1/\lambda^3 \\ 1/\lambda^2 \\ 1/\lambda \\ 1 \end{bmatrix} \tag{29}$$

approaches an eigenvector of $MM^\dagger$ with eigenvalue zero as $N \to \infty$.

For step 2, start with the fact that the ground state is unique when N and λ are finite, because then $M^\dagger M$ does not have any eigenvectors with eigenvalue zero when N is finite.[34] The unitary operator S that implements the flip-all-bits symmetry (equation (4)) commutes with the hamiltonian, so the unique ground state must also be an eigenstate of S. The operator S anticommutes with every Z_n, so it anticommutes with each of the Clifford operators A_n and B_n defined in section 15, which in turn implies that it anticommutes with each of the fermion operators $c(u)$ defined in section 17. Use this to see that the state $c^*(u)|g\rangle$ is also an eigenstate of S, but with the opposite eigenvalue (same magnitude, opposite sign). For convenience, write c_0 as an abbreviation for $c(u_0)$ when u_0 is the eigenvector of $M^\dagger M$ for which $m(u_0) \to 0$ as $N \to \infty$. We just learned that $|g\rangle$ and $c_0^*|g\rangle$ are both eigenstates of S with opposite eigenvalues (same magnitude, opposite sign), so the two mutually orthogonal states

$$|g_\pm\rangle \equiv \left(1 \pm c_0^*\right)|g\rangle \tag{30}$$

are exchanged with each other by S. In the limit $N \to \infty$ with $\lambda > 1$, these two states are both ground states, so we have two ground states that are exchanged with each other by the symmetry. This completes step 2.

To address step 3, we need to show that the two states (30) are not mixed with each other by any local observables.[35] The anticommutation relations (21)

[34] This will be confirmed in sections 19-20.

[35] In symbols: we need to show that $\langle g_+|Q|g_-\rangle = 0$ and $\langle g_-|Q|g_+\rangle = 0$ for any local observable Q.

and equation (22) imply that the states $|g_\pm\rangle$ are both eigenstates of the operator $c_0 + c_0^*$, with opposite eigenvalues:

$$(c_0 + c_0^*)|g_\pm\rangle = \pm|g_\pm\rangle. \tag{31}$$

Equation (20) implies

$$c_0 + c_0^* = -\sqrt{2}A^\dagger \tilde{u}_0.$$

An earlier paragraph showed that the vector $\tilde{u}_0$ approaches the form (29) as $N \to \infty$, so the operator $c_0 + c_0^*$ approaches the form

$$c_0 + c_0^* \to -\sqrt{2}\sum_{n=1}^{N} \frac{A_n \lambda^n}{\lambda^N} \tag{32}$$

as $N \to \infty$. Now recall the definition of A_n in equations (8)-(9): it is a product of qubit operators associated with lattice sites $\geq n$ only. Therefore, for any given finite value of n, the terms in the sum (32) involving qubit operators at lattice sites $k \leq n$ all go to zero, because λ^k/λ^N goes to zero for all $k \neq n$ when n is held fixed and $N \to \infty$.[36] This implies that when $N \to \infty$, the operator $c_0 + c_0^*$ commutes with all local observables. Combined with equation (31) this implies that local observables cannot mix the two ground states $|g_\pm\rangle$ with each other. This completes step 3.

Altogether, this shows that in the limit $N \to \infty$, the model with hamiltonian (2) is in the SSB phase for all $\lambda > 1$.

For $\lambda < 1$, the model is in the symmetric phase. This can be proved by showing that all of the $m(u)$s approach nonzero limits as $N \to \infty$ when $\lambda < 1$ (sections 19-20). Then the lowest energy in (23) is attained only when the set V is empty. That implies that the ground state is unique, so it must be an eigenstate of the operator S that implements the flip-all-bits symmetry.

[36] This is why the operators A, B were defined using a product of qubit operators that extends to the right (toward the index N) instead of to the left (toward the index 0). That matters because we're taking the limit as the lattice becomes infinite in only one direction, namely to the right.

19 The energy spectrum, part 1

As explained in section 17, we can calculate the complete energy spectrum by determining the eigenvalues of the matrix (24), which can also be written like this:

$$M^\dagger M = (1+\lambda^2)I - \lambda J \tag{33}$$

with

$$J \equiv T^\dagger + T + \begin{bmatrix} \lambda & 0 & 0 & \cdots \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & \\ \vdots & & & \ddots \end{bmatrix}.$$

For $N = 5$, this is

$$J = \begin{bmatrix} \lambda & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

The eigenvectors of $M^\dagger M$ are the same as those of J.

To find eigenvectors of J, consider the ansatz

$$v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix}$$

with components

$$v_n = \beta z^n - \frac{1}{\beta z^n}, \tag{34}$$

where β and z are complex numbers to be determined. This ansatz automatically satisfies all but the first and last rows of the eigenvector equation

$$Jv = \left(z + \frac{1}{z}\right) v, \tag{35}$$

so the eigenvalue is $z + 1/z$. The first and last rows of equation (35) are

$$\begin{aligned} \lambda\left(\beta z - \frac{1}{\beta z}\right) + \beta z^2 - \frac{1}{\beta z^2} &= \left(z + \frac{1}{z}\right)\left(\beta z - \frac{1}{\beta z}\right) \\ \beta z^{N-1} - \frac{1}{\beta z^{N-1}} &= \left(z + \frac{1}{z}\right)\left(\beta z^N - \frac{1}{\beta z^N}\right) \end{aligned} \tag{36}$$

which we can use to determine the values of β and z. After expanding the right-hand sides, equations (36) reduce to

$$\begin{aligned} \lambda\left(\beta z - \frac{1}{\beta z}\right) &= \beta - \frac{1}{\beta} \\ 0 &= \beta z^{N+1} - \frac{1}{\beta z^{N+1}}. \end{aligned} \tag{37}$$

The second equation may be used to express b in terms of z:

$$\beta = \frac{\pm 1}{z^{N+1}},$$

and using this to eliminate β from the first equation in (37) gives

$$\lambda\left(z^N - \frac{1}{z^N}\right) = z^{N+1} - \frac{1}{z^{N+1}}. \tag{38}$$

20 The energy spectrum, part 2

To find values of z that satisfy equation (38), consider two possibilities:

- z is a positive real number, so $z = e^\theta$ for some real number θ.
- z is a complex number with magnitude 1, so $z = e^{i\theta}$ for some real number θ.

For the first possibility, equation (38) becomes

$$\lambda \sinh(N\theta) = \sinh\big((N+1)\theta\big). \tag{39}$$

The trivial solution $\theta = 0$ does not give an eigenvector, because in that case $z = \beta = 1$, which makes the ansatz (34) zero. The hyperbolic sine function, sinh, has a monotonically increasing magnitude as a function of $\theta > 0$, so equation (39) does not have any other solutions unless $\lambda > 1$, in which case has only one solution. Equation (38) shows that this one solution approaches

$$z \to \lambda$$

as $N \to \infty$, so the corresponding eigenvalue of J approaches $z + 1/z \to \lambda + 1/\lambda$, which means that the corresponding eigenvalue of (33) approaches zero. This agrees with the result that was obtained in step 1 in section 18.

For the second possibility, $z = e^{i\theta}$, equation (38) becomes

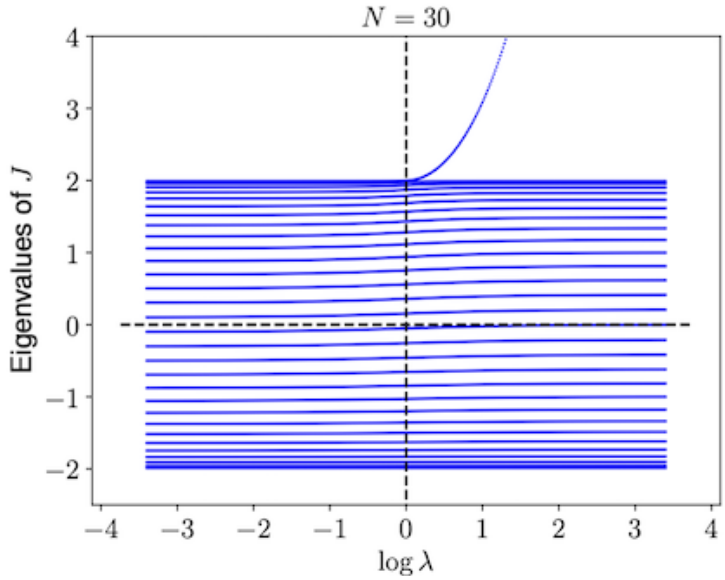
$$\lambda \sin(N\theta) = \sin\big((N+1)\theta\big). \tag{40}$$

Any nonzero solutions of this equation give an eigenvalue of J equal to $z + 1/z = 2\cos\theta$, whose magnitude cannot exceed 2.

Are these the only eigenvalues of (35)? We could answer this by counting the number of solutions of (38), because we know that J must have N eigenvalues altogether.[37] The solution-counting approach is tricky, though, so I'll use a different

[37] If we could determine that equation (40) has exactly N solutions for $\lambda \le 1$ and exactly $N-1$ solutions for $\lambda > 1$, then we would know that we have found all of the eigenvalues and eigenvectors of J.

approach: I'll use a computer to determine the eigenvalues of the matrix J and graph them all as a function of λ for several different values of N. The goal is to discover if J has any other eigenvalues that are not included in the ones we already found analytically. Here's an example:[38]



This picture shows the eigenvalues of J, computed numerically, for a lattice with $N = 30$ sites, over the range $1/30 < \lambda < 30$. The horizontal axis is $\log \lambda$ so that the region with $\lambda < 1$ gets the same attention as the region with $\lambda > 1$. With the exception of one eigenvalue that approaches $\lambda + 1/\lambda$ for large N when $\lambda > 1$, all of the other eigenvalues have magnitudes ≤ 2. This is good evidence that the matrix (33) doesn't have any eigenvalues other than the ones we already found analytically, namely:

- eigenvalues of the form $1 + \lambda^2 - 2\lambda \cos(\alpha)$, and
- one eigenvalue that approaches zero for $N \to \infty$ when $\lambda > 1$.

The complete spectrum of the hamiltonian (2) may then be obtained by using these eigenvalues of the matrix (33) in equation (23).

[38]The Python script used to generate this picture is posted here: https://cphysics.org/extras/81040b.html

21 The self-dual model

Section 3 defined two different hamiltonians. The first version, equation (2), was the subject of equations (12)-(20). Starting in this section, we'll study the other version, equation (3). Intuitively, the difference between the two models should become irrelevant when $N \to \infty$, because they differ only in how they treat the Nth qubit. The motive for studying both versions was previewed in section 8.

As previewed in section 8, the energy spectrum of the hamiltonian (3) is invariant under the replacement $\lambda \to 1/\lambda$, up to a rescaling of the energy scale by an factor of λ. This property of the energy spectrum is called **self-duality**. To prove this, temporarily append an extra site to the left end[39] of the lattice, so that the allowed index-values are

$$0,\ 1,\ 2,\ ...,\ N.$$

The hamiltonian is defined by equation (3), repeated here for convenience:

$$\hat{H} = -\sum_{n=1}^{N-1} X_n - \lambda \sum_{n=1}^{N-1} Z_n Z_{n+1}. \tag{41}$$

This hamiltonian doens't involve the extra qubit, but the extra qubit allows us to define these new qubit operators that are dual to the original ones:

$$\begin{aligned} \tilde{X}_n &\equiv Z_n Z_{n+1} && \text{for } 1 \le n \le N-1 \\ \tilde{Z}_n &\equiv \prod_{k=0}^{n} X_k && \text{for } 0 \le n \le N. \end{aligned} \tag{42}$$

This relationship is nonlocal, but the algebra generated by the $\tilde{X}$s and $\tilde{Z}$s is isomorphic to the one generated by the original operators X and Z. The hamiltonian (41) can be written in terms of the dual operators like this:

$$\hat{H} = \lambda \left(-\sum_{n=1}^{N-1} \tilde{X}_n - \frac{1}{\lambda} \sum_{n=1}^{N-1} \tilde{Z}_{n-1} \tilde{Z}_n \right). \tag{43}$$

[39] This directional language assumes that the index labeling the lattice sites increases from left to right.

This looks like (41) with the replacements $X \to \tilde{X}$ and $Z \to \tilde{Z}$ and $\lambda \to 1/\lambda$, except that one of the sums is shifted and except for the overall factor of λ. The overall factor of λ doesn't matter, because it just redefines the unit of energy. The shifted sum doesn't matter, either: the original hamiltonian (41) and the dual hamiltonian (43) both include one ZZ-term for each X term, the only difference being that the ZZ term is to the right (for (41)) or left (for (43)) of the corresponding X term. We can map one to the other just by relabeling the index-values

$$(0, 1, 2, ..., N) \to (N, ..., 2, 1, 0),$$

which clearly cannot affect the hamiltonian's eigenstates or eigenvalues. This shows that the model with hamiltonian (41) is self-dual even when N is finite.

This is a property of the hamiltonian (41), so the extra qubit that we temporarily appended to the lattice (namely the $n = 0$ qubit) isn't really needed. It adds an extra bit to the binary numbers b in section 2, effectively replacing each eigenstate with a pair of eigenstates having the same eigenvalue, distinguished from each other only by the value of the extra bit. Aside from this trivial doubling, the extra qubit has no effect on the hamiltonian's eigenstates or eigenvalues, so the extra bit will be omitted from now on.

22 A few paradoxes

Intuitively, predictions obtained using the self-dual hamiltonian (3) should agree with those using the left-right symmetric hamiltonian (2) when $N \to \infty$, because they differ only in how they treat the Nth qubit. In particular, they should both become self-dual when $N \to \infty$. The results derived earlier for the the left-right symmetric hamiltonian (2) might seem incompatible with self-duality, though. I'll express this as a few paradoxes:

- The **two-phases paradox**: For the hamiltonian (2), for $N = \infty$, the ground state respects the flip-all-bits symmetry when $\lambda < 1$ but not when $\lambda > 1$.
- The **number-of-ground-states paradox**: For the hamiltonian (2), the lowest energy has *two* corresponding eigenstates for $\lambda > 1$ but only *one* corresponding eigenstate for $\lambda < 1$.
- The **spectrum shape paradox**: The pictures in section 13 show that the second-lowest energy diverges away from the lowest energy as λ decreases from 1 to 0 but stays close to the lowest energy as λ increases from 1 to ∞.

How can these features of the hamiltonian (2) be consistent with the self-duality of the hamiltonian (3), if their predictions become identical when $N \to \infty$?

The two-phases paradox is resolved by the fact that the relationship (42) between the original qubit operators X, Z and the dual qubit operators $\tilde{X}, \tilde{Z}$ is nonlocal. Self-duality is a property of the *energy spectrum* and of the *number* of energy eigenstates associated with each energy eigenvalue, but it does not preserve the association between observables and regions of space:[40] the original flip-all-bits operator (4) is transformed to a single $\tilde{Z}$-operator.

Section 23 illustrates how the number-of-ground-states paradox is resolved, and section 24 illustrates how the spectrum shape paradox is resolved.

[40] Cotler *et al* (2017) shows that the structure of the hamiltonian as a sum of local observables is closely related to the structure of the energy spectrum, but that relationship is only sensitive to the *equivalence class* of the hamiltonian's local structure.

23 The zero- and infinite-coupling cases

When $\lambda = 0$, the self-dual hamiltonian (41) reduces to

$$-\hat{H}_X = -\sum_{n=1}^{N-1} X_n. \tag{44}$$

The ground state of (44) would be unique (section 9), except that the sum in (44) doesn't include the Nth qubit.[41] Because of that unused qubit, the hamiltonian (44) actually has *two* linearly independent ground states when $\lambda = 0$, namely

$$\frac{1 \pm Z_N}{2} \sum_b |b\rangle, \tag{45}$$

where the operators $(1 \pm Z_N)/2$ project the unused qubit to the bit-value 0 or 1, respectively. The two ground states (45) are distinguished from each other only by observables that involve the unused qubit.

When $\lambda \to \infty$, the hamiltonian (41) approaches

$$-H_Z = -\sum_{n=1}^{N-1} Z_n Z_{n+1}, \tag{46}$$

up to an overall factor of λ. In this case, the lowest energy is attained by two linearly independent ground states, just like in section 10.

This shows that the cases $\lambda = 0$ and $\lambda \to \infty$ both have the same number of linearly independent ground states, namely two. Even more, when $\lambda = 0$, we can choose a basis for the two-dimensional space of ground states in which the chosen basis states (namely (45)) are exchanged with each other by the flip-all-bits symmetry, just like we can when $\lambda \to \infty$. However, the cases $\lambda = 0$ and $\lambda \to \infty$ differ from each other in one crucial respect. In the case $\lambda = 0$, in the limit $N \to \infty$,

[41] As promised at the end of the previous section, the Hilbert space no longer includes the 0th qubit.

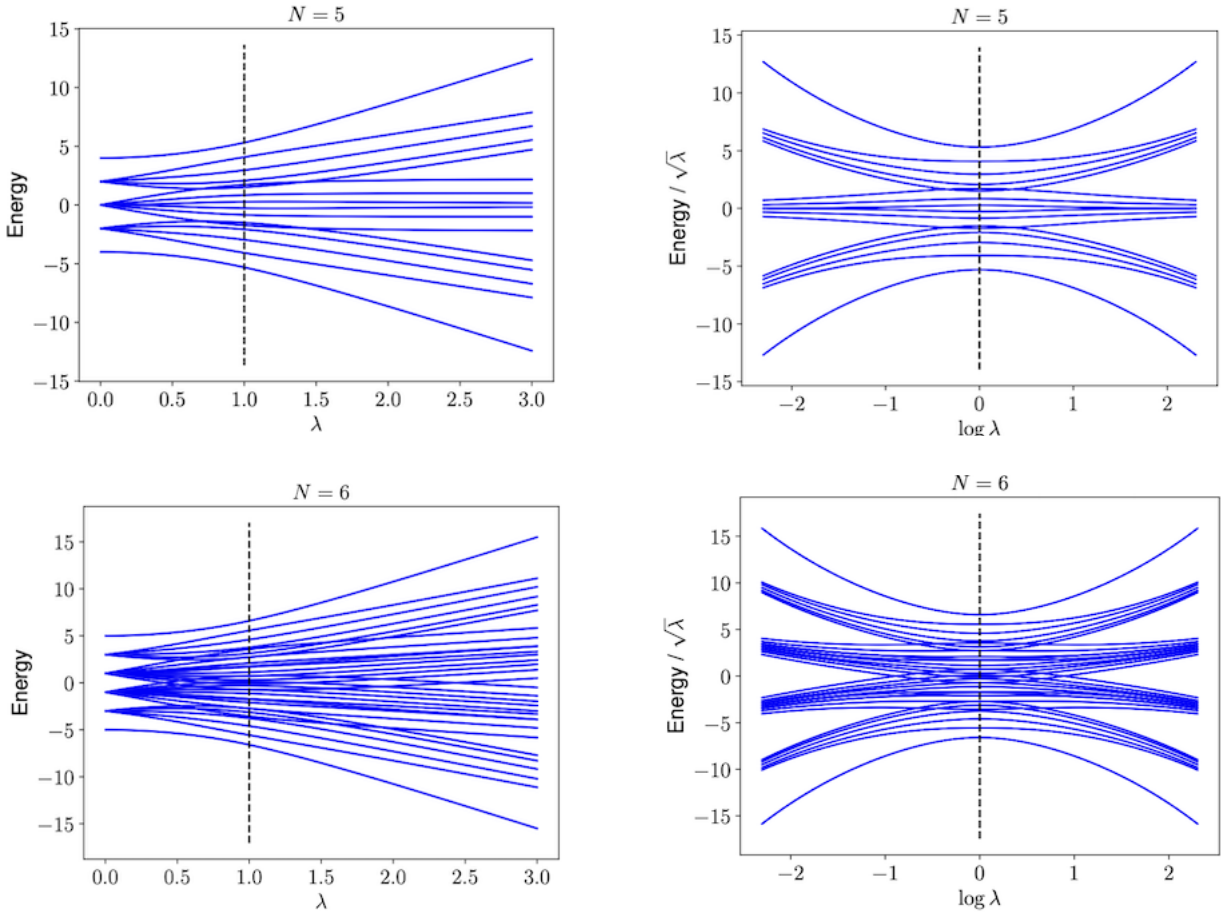
the bit that breaks the flip-all-bits symmetry – namely the Nth bit – gets pushed out to spatial infinity, where it is beyond the reach of any local observables. The result is that the ground state is invariant under the flip-all-bits symmetry *as far as any local observables can tell*. In contrast, in the case $\lambda \to \infty$, all of the bits break the symmetry, so the fact that the symmetry is broken remains visible to local observables even when $N = \infty$. In both cases, $\lambda = 0$ and $\lambda \to \infty$, the two basis states that are exchanged with each other by the flip-all-bits symmetry cannot be mixed with each other by any local observables when $N = \infty$, so in each case we get two superselection sectors. Here's the key: we must choose *one* of those two superselection sectors. In the case $\lambda = 0$, they are identical to each other as far as local observables can tell. In the case $\lambda \to \infty$, they are not.[42]

We only considered the extreme cases $\lambda = 0$ and $\lambda \to \infty$ here, but this already illustrates how the number-of-ground-states paradox is resolved. The next section studies the self-dual model for arbitrary values of λ.

[42] Actually, that's only true if the system of qubits is regarded as one part of a larger system. In a pretend universe described entirely by the quantum Ising model, with nothing else at all, the choice between the all-0s state and the all-1s state would be purely a matter of convention. A similar statement holds for *any* truly perfect symmetry of *any* truly complete model. The SSB phase is still distinct from the symmetric phase, but different superselection sectors related to each other by symmetry are effectively equivalent to each other.

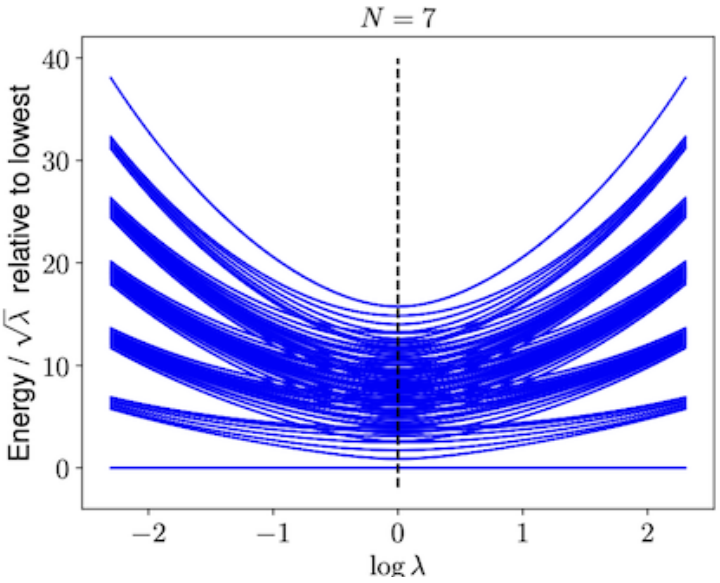
24 Energy spectrum on small lattices

When $N \to \infty$, the case $\lambda = 1$ is special in the self-dual model, just like it was in the left-right symmetric model. To highlight what happens when $\lambda = 1$, this section shows a few examples of the energy spectrum, determined numerically, for small values of N.[43] The pictures on the left side show the energies as a function of λ, like in section 13 but for the self-dual hamiltonian (41). The pictures on the right side show the energies rescaled by $\sqrt{\lambda}$ as a function of $\log\lambda$, so that the self-duality property $\lambda^{-1/2}E(\lambda) = \lambda^{1/2}E(1/\lambda)$ is evident.



[43] The source code used to generate these results is the same as in footnote 18.

Here's the $N = 7$ case, this time showing the energies relative to the lowest energy:



This highlights something special about the critical point $\lambda = 1$ ($\log \lambda = 0$): when $N \to \infty$, the gap between the the infinum of the energy spectrum and the continuum of higher energies shrinks to zero. As explained in Kogut (1979), this phenomenon plays an important role in understanding how a relativistic quantum field theory (QFT) with exact Poincaré symmetry – and even exact conformal symmetry – can emerge in the appropriate limit from a model defined on a discrete lattice.

This also illustrates how the spectrum shape paradox (section 22) is resolved. When $N \to \infty$, the spectrum is gapless at $\lambda = 1$. This is true no matter which hamiltonian is used, (2) or (3). For the hamiltonian (2), the second-lowest energy diverges away from the lowest energy as λ decreases from 1 to 0. As λ increases from 1 to ∞, the energy that would be second-lowest when N is finite becomes identical to the lowest energy when $N = \infty$, so it is no longer the *second*-lowest energy. For $\lambda > 1$, the second-lowest energy when $N = \infty$ corresponds to the *third*-lowest energy when N is finite, and that energy level diverges away from the lowest energy as λ increases from 1 to ∞, just like self-duality says it should. The fact that the spectrum becomes gapless at $\lambda = 1$ makes this bait-and-switch possible.

25 References

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